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Published in:
2nd IWA/WEF Wastewater Treatment Modelling Seminar

Publication date:
2010

[Link back to DTU Orbit](#)

Citation (APA):
Sin, G., Ruano, M. V., Neumann, M. B., Ribes, J., Gernaey, K., Ferrer, J., Loosdrecht, M. C. M. V., & Gujer, W. (2010). Sensitivity analysis in the WWTP modelling community – new opportunities and applications. In *2nd IWA/WEF Wastewater Treatment Modelling Seminar*

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Sensitivity analysis in the WWTP modelling community – new opportunities and applications

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Abstract

A mainstream viewpoint on sensitivity analysis in the wastewater modelling community is that it is a first-order differential analysis of outputs with respect to the parameters – typically obtained by perturbing one parameter at a time with a small factor. An alternative viewpoint on sensitivity analysis is related to uncertainty analysis, which attempts to relate the total uncertainty in the outputs to the uncertainty in the inputs. In this paper we evaluate and discuss two such sensitivity analysis methods for two different purposes/case studies: (i) Applying sensitivity analysis to a plant design (BSM1 plant layout) using Standardized Regression Coefficients (SRC) and (ii) Applying sensitivity analysis to help fine-tuning a fuzzy controller for a BNPR plant using Morris Screening. The results obtained from each case study are then critically discussed in view of practical applications of sensitivity analysis in day-to-day engineering projects.

INTRODUCTION

Modelling of wastewater treatment plants (WWTPs) has moved beyond academic circles to engineering practice where it serves to tackle complex and challenging problems of wastewater treatment technology. WWTP models are used for many applications/purposes including plant design, optimisation and control. The model predictions are not free from uncertainty as these models are an approximation of reality (abstraction), and are typically built on a considerable number of assumptions.

Uncertainty analysis is concerned with quantifying the output uncertainty (or prediction uncertainty of models) caused by various sources of uncertainty present in the input. While, the sensitivity analysis attempts to quantify and therefore identify the individual contribution of input uncertainty on the output uncertainty. This definition is in contrast with most sensitivity analysis studies done in the field of wastewater treatment which are local and use a differential analysis of outputs with respect to the parameters. This is understandable as this concept of sensitivity analysis is related to the control/model identification theory, which has long been part of the research agenda in this community. However, the above-mentioned definition called global sensitivity analysis is pioneered by applied statisticians and relates to variance decomposition theory in general (Saltelli *et al.*, 2004).

In this study, we demonstrate and discuss two applications of global sensitivity analysis. The first application deals with a plant design example, for which we have selected the benchmark (BSM1) plant layout and its operational and influent characterisation as case study (Copp, 2002). The purpose for the sensitivity analysis is to answer the following question: given a plant layout, an operational configuration and an influent profile, what are the most significant inputs (biokinetic parameters, influent fractions, aeration parameters, etc) contributing to the uncertainty of the key plant performance criteria: effluent quality, sludge production and energy consumption. The model set-up, the characterisation of input

uncertainty and the uncertainty analysis were performed in a previous study (Sin *et al.*, 2009). To this end, Monte Carlo simulations combined with the linear regression method as a sensitivity measure (also known as Standardized regression coefficients) (Saltelli *et al.*, 2004) is used.

The second application deals with fine-tuning of a fuzzy controller applied to WWTP plant operation. In a previous work, a systematic approach based on local sensitivity analysis was developed and evaluated for an aeration control system implemented in a WWTP performing biological phosphorus and nitrogen removal (Ruano *et al.*, 2009). In this case study, a global sensitivity analysis is applied aimed at screening the most influential parameters of the fuzzy-control systems to be used in the fine-tuning procedure. The Morris method of Elementary Effects (EEi) (Morris, 1991) was used as sensitivity analysis method.

MATERIAL AND METHODS

Case study 1:

BSM1 plant layout, simulation strategy and plant performance evaluation

The BSM1 plant is a pre-denitrification system for nitrogen removal. The activated sludge unit, modelled using the Activated Sludge Model no 1 (ASM1, Henze *et al.*, 2000) consists of 5 compartments, in which the first two are anoxic with a total volume of 2000 m³, while the last three are aerated with a total volume of 3999 m³. The settling unit, modelled using the Takács settling model, is a non-reactive secondary settler with a volume of 6000 m³ (area of 1500 m², depth of 4 m) subdivided into 10 layers. For further details on the BSM1 the reader is referred to the IWA Task Group on Benchmarking of Control Strategies for WWTPs (<http://www.benchmarkwwtp.org/>) and Copp (2002). The model of the BSM1 layout – modified with MLSS controller– is implemented and simulated in Matlab / Simulink (Sin *et al.*, 2009).

Sensitivity Analysis

Monte Carlo procedure

For notational convenience, the WWTP model structure is represented by \mathbf{f} , the state vector by \mathbf{x} , the input variables by \mathbf{u} , the input parameter vector by $\boldsymbol{\theta}$, the output vector of the target variables by \mathbf{y} (target variables \mathbf{y} being aggregate measures $g(\mathbf{x})$ of the states \mathbf{x}), and time is represented by t :

$$\begin{aligned} \frac{d\mathbf{x}}{dt} &= \mathbf{f}(\mathbf{x}, \mathbf{u}, t, \boldsymbol{\theta}), \quad (\mathbf{x}_0) = \mathbf{x}_0; \\ \mathbf{y} &= \mathbf{g}(\mathbf{x}(t)) \end{aligned} \tag{Eq. 1}$$

Following the selection of an appropriate mathematical model structure, uncertainty analysis using Monte Carlo Simulation involves the following steps: (1) Specifying input uncertainty, (2) Sampling input uncertainty, (3) Propagating input uncertainty through \mathbf{f} to obtain prediction uncertainty for \mathbf{y} , and (4) Representation and interpretation of results.

Standardized Regression coefficients(SRC)

The standardized regression coefficients are obtained by performing a linear regression on each of the model outputs obtained from the Monte Carlo simulation:

$$sy_k = b_{0k} + \sum_{i=1}^I b_{k,i} \cdot \theta_i + \varepsilon_k \quad \text{for } k = 1, 2, \dots, K \tag{Eq. 2}$$

\mathbf{sy}_k is a vector of scalar values for the k^{th} model output, \mathbf{b}_k is a vector of coefficients, $\boldsymbol{\theta}$ is a matrix of parameter values (the sampling matrix) and $\boldsymbol{\varepsilon}_k$ is the error vector of the regression model. Equation 2 can also be written in a dimensionless form using the corresponding means

(μ_{sy_k}, μ_θ) and standard deviations $(\sigma_{sy_k}, \sigma_\theta)$ of the outputs and the parameters respectively (Saltelli *et al.*, 2004):

$$\frac{sy_k - \mu_{sy_k}}{\sigma_{sy_k}} = \beta_k \frac{\theta - \mu_\theta}{\sigma_\theta} + \varepsilon_k \quad \text{Eq. 3}$$

β_k is a vector of standardized regression coefficients (SRC) of the parameters that correspond to the k^{th} model output, y_k .

Case study 2

WWTP and control system description

The fuzzy logic based control system was implemented to control the aeration in a nutrient removing WWTP based on a modified UCT scheme (see Figure 1).

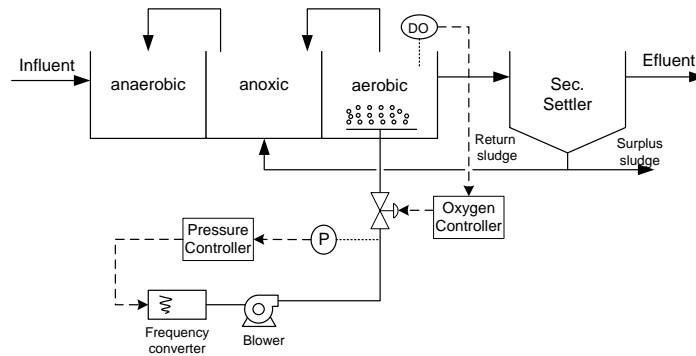


Figure 1. Flow diagram of the control system applied to a modified UCT process.

The main objective of this control system is to control the oxygen in the plant by using two controllers, one for dissolved oxygen and one for air pressure. The first controller manipulates the air valve opening according to DO concentration, while the rotational speed of the blower is manipulated to reach the discharge pressure set point. As each control valve is governed by an independent DO controller, the air pressure controller is implemented in order to enhance the control system when there is more than one air valve in the same air pipeline. This controller aims at obtaining the ideal situation where the movement of one valve, which is governed by its DO controller, does not affect the air flow rate through the other valves in the same air pipeline. However, it should be mentioned that there is only one DO controller in this case study in order to simplify the aeration control system. For the DO controller the input variables are the oxygen error (*OE*) and the accumulated oxygen error (*AOE*) and the output variable is the increment/decrement of the air valve opening (*IV*). For the air pressure controller the input variables are the pressure error (*PE*) and the accumulated pressure error (*APE*) and the output variable is the increment/decrement of the rotational speed of the blower (*IB*), which is governed by a frequency converter. Both controllers are fuzzy logic based controllers, which consist of five stages. The first stage and the last stage are the same for both controllers. Stage 1 is the input stage (the measured or calculated variables are input to the controller) and stage 5 is the output stage. In the stage 2, so called *fuzzification*, the data collected from on-line sensors are converted into linguistic variables (fuzzy set), represented by membership functions (Gaussian shape in this study). In the stage 3 a set of rules (so called *inference engine*) are applied to the fuzzy set obtained in the stage two. The output linguistic variables are obtained in this stage by the Max-Prod operator, following the Larsen's fuzzy inference method (Larsen, 1980). These linguistic variables are converted into numerical control actions in the stage four, which is called *defuzzification*. In order to obtain a single output value from our fuzzy linguistic set, the Height Defuzzifier method was employed (Mendel, 1995), which only uses the centre of the Gaussian defuzzification membership

functions. The total number of parameters of both controllers comes from the different stages of the fuzzy logic based controllers, mainly derived from the *defuzzification* and *fuzzification* steps (Ruano et al., 2009). Both controllers use three Gaussian membership functions to fuzzificate each input (“High Negative”, *HN*; “Low Negative”, *LN*, and “Low Positive”, *LP*) which gives a total of 12 membership functions from both fuzzification stages; and four to defuzzificate each output (“High Negative”, *HN*; “Low Negative”, *LN*; “Low Positive”, *LP*, and “High Positive”, *HP*) which gives a total of 8 membership functions from both defuzzification stages. As each Gaussian curve is defined by two parameters (centre, *c*, and amplitude, *a*), the control system has a total of 24 parameters corresponding to the *fuzzification* stages. In contrast, for the *defuzzification* stages only the centres are used giving a total of 8 parameters. Including the response time of the control system (*RT*), i.e. time interval between two control actions, a total number of 33 parameters need to be adjusted. In order to identify the parameters of this control system, acronyms for each parameter have been used. These acronyms are constructed as follows: “abbreviation of input variable”+ “c/a”+“fuzzification/defuzzification membership function abbreviation”. For instance, the acronym *OEaHN* means the amplitude of the High Negative membership function for the input variable Oxygen Error; and the acronym *IVcLN* means the centre of the Low Negative membership function for the output variable Increment air Valve opening.

In order to decrease the computational demand, in this case study we simplified the control system to 17 parameters assuming symmetric behaviour of the membership functions defined for each fuzzy variable. This symmetric behaviour involves that the amplitude for the three Gaussian membership functions is the same and their centres are equidistant. This control structure is the simplest one that can be implemented in a WWTP, as the oxygen concentration is controlled in only one reactor. When more aerobic reactors are to be controlled, the number of parameters will increase proportionally. As an example, this control system has recently been implemented in Denia WWTP (Denia, Spain) (Ribes *et al.*, 2007), with 9 different oxygen variables and one pressure (as the same group of blowers are used to aerate the whole system). Hence, reducing the number of tuning parameters in this kind of controllers is essential.

The fuzzy controller and the WWTP model were implemented and simulated using the WWTP simulation software DESASS (Ferrer *et al.*, 2008). This software includes the plant-wide model Biological Nutrient Removal Model n° 1 (BNRM1, Seco et al., 2004). The simulation strategy consisted of a steady-state simulation to obtain proper initial conditions followed by 28 days dynamic simulations. The last 14 days were considered to evaluate the performance of the control system. The standardised influent file for dry weather proposed by Copp (2002) was used in this study. The Integral Absolute Error (IAE, integral of the absolute value of the time dependent error function) for each controller (Oxygen and Pressure) was selected as output measure. So in this study *IAEO* and *IAEP* are the output variables.

Sensitivity analysis

Morris screening

The method of Morris (1991) evaluates the so called distribution of Elementary Effects (EE) of each input factor to model outputs, from which basic statistics are computed to derive sensitivity information. This distribution function is denoted as F_{jk} , which stands for the distribution of the effects of the j^{th} input parameter on the k^{th} output. The EE_{jk} attributable to each input parameter is obtained from the following differentiation of model output, sy_k , with respect to the input, θ_j :

$$EE_{jk} = \frac{sy_k(\theta_1, \theta_2, \theta_j + \Delta, \dots, \theta_M) - sy_k(\theta_1, \theta_2, \theta_j, \dots, \theta_M)}{\Delta} \quad \text{Eq. 4}$$

Where Δ is a predetermined perturbation factor of θ_j , $sy_k(\theta_1, \theta_2, \theta_3, \theta_j, \dots, \theta_M)$ is the scalar model output evaluated at input parameters $(\theta_1, \theta_2, \theta_3, \theta_j, \dots, \theta_M)$, while $sy_k(\theta_1, \theta_2, \theta_3, \theta_j + \Delta, \dots, \theta_M)$ is the scalar model output corresponding to a change in θ_j . Each input parameter, θ_j , can only take values corresponding to (a predefined set of) p levels within its range. The calculations of the elementary effects, EE_{jk} , is replicated r times, at randomly sampled points in the input space, leading to a distribution of EE_{jk} used to infer a global sensitivity measure. To do that, an effective one-factor-at-a-time (OAT) design has been developed (Morris, 1991). As in the Monte-Carlo procedure shown in case study 1, the input uncertainty must be specified.

In this case study, the scaled elementary effects SEE_{jk} proposed by Sin and Gernaey (2009) were applied. The resulting elementary effects of each output variable (IAEO and IAEP) show the sensitivity of each controller separately (oxygen and pressure controller, respectively). However both controllers must be tuned as a global MIMO (Multiple Input Multiple Output) control system. Thus sensitivity analysis aiming at selecting the most influential parameters in this MIMO system was carried out giving an equal weight contribution of the scaled elementary effects obtained from both output variables. The scaled elementary effect of the j^{th} input parameter on the weighted contribution of both output variables was calculated as follows:

$$SEE_j = \frac{EE_{jIAEO}}{\sigma_{IAEO}} + \frac{EE_{jIAEP}}{\sigma_{IAEP}} \quad \text{Eq. 5}$$

Where σ_{IAEO} and σ_{IAEP} are the standard deviations of the corresponding output variables. Once the distribution of the scaled elementary effects is obtained, the sensitivity measures mean (μ) and standard deviation (σ) of each F_{jk} are determined. In order to identify the influential parameters these sensitivity measures were then interpreted using the graphical approach proposed by Morris. In this approach the values of the μ and the σ obtained for all the F_{jk} distributions are displayed together with two lines corresponding to $\mu_i = \pm 2SEM_i$, where the SEM_i represents the standard error of the mean that can be estimated as $SEM_i = \sigma_i / \sqrt{r}$. Parameters with low μ and low σ are deemed as non-influential.

One issue of particular interest is the selection of the resolution, p , and number of trajectories, r . Cropp and Braddock (2002) pointed out that a good choice of the sample size (r) is more critical for obtaining a good estimate of the effects than the resolution (p). In this case study, an optimal setting of r was searched with a constant resolution of $p=8$. To this end, the number of repetitions of elementary effects calculations (r) for each distribution F_{jk} was increased until the influential parameters remained more or less stable, i.e. the type II error was minimised (type II error: identifying an important factor as insignificant). Once the r_{opt} was found, the graphical Morris approach was used to find the non influential parameters.

RESULTS AND DISCUSSIONS

Case study 1: Application of sensitivity analysis to BSM1 plant design

The time-series data (dynamic simulations) obtained from the Monte Carlo simulations were averaged flow proportionally for the four plant performance criteria considered: effluent nitrate, effluent ammonia, sludge production and aeration energy requirement. Linear regression models were then fitted to each of the averaged plant performance criteria hence resulting in four linear regression models - essentially predicting the plant performance criteria as linear coefficients of the BSM1 model parameters. The corresponding coefficients

of the linear models are scaled to obtain the standardized regression coefficients (SRC) which are shown in Table 1 together with their importance rank (i.e. the higher the rank, the higher the importance). It is noted that the linear model determination coefficients (R^2) are all found to be higher than 0.7. This means that the SRC can explain more than 70% of the output variance making them a useful measure for sensitivity.

Table 1 Standardized regression coefficients (SRCs) obtained for the 4 linear models and their corresponding ranks. Sensitive parameters ($\text{abs}(\text{SRC}) > 0.1$) shown in **bold** (for definition of symbols please refer to <http://www.benchmarkwwtp.org/>).

	Effluent NO_3		Effluent NH_4		Sludge production		Aeration energy	
R^2	0.88		0.71		1.00		0.77	
Parameter	SRC	rank	SRC	rank	SRC	rank	SRC	rank
μ_H	-0.01	30	-0.03	19	0.00	20	0.03	18
K_S	0.02	25	0.02	23	-0.01	17	-0.01	27
K_{OH}	-0.28	5	-0.07	13	0.00	22	-0.08	10
K_{NO}	0.06	19	0.03	20	0.00	31	0.02	20
b_H	-0.01	29	-0.02	22	-0.06	7	0.08	11
μ_A	0.05	21	-0.19	6	0.01	18	0.00	28
K_{NH}	-0.10	14	0.30	3	-0.01	16	0.00	33
K_{OA}	-0.02	26	0.18	8	0.00	24	0.00	31
b_A	-0.06	20	0.24	5	-0.01	13	0.01	23
η_g	-0.16	10	-0.05	15	0.00	21	-0.03	15
k_a	0.08	17	0.01	32	0.00	29	0.04	13
k_h	-0.14	12	0.02	25	-0.01	12	-0.03	16
K_X	0.09	15	0.01	26	0.01	14	0.02	21
η_{hyd}	-0.33	4	-0.01	31	0.00	30	-0.11	9
Y_H	0.21	7	0.09	12	0.32	3	-0.30	2
Y_A	0.00	33	-0.01	29	0.01	10	-0.01	24
f_P	-0.01	28	0.09	11	0.10	4	-0.15	6
i_{XB}	-0.26	6	-0.13	10	-0.01	11	-0.12	8
i_{XP}	0.00	32	-0.02	24	0.00	25	0.00	29
X_{2TSS}	-0.04	24	0.43	1	0.84	1	-0.21	5
f_{SI}	0.16	9	-0.05	16	-0.09	5	-0.03	17
f_{SS}	-0.36	2	0.00	33	0.00	26	-0.12	7
f_{XI}	0.48	1	0.18	7	0.44	2	-0.28	3
f_{XBH}	0.04	23	0.01	30	0.09	6	-0.07	12
i_{SND_SS}	0.01	31	-0.01	28	0.00	28	0.01	25
i_{XND_XS}	-0.01	27	-0.01	27	0.00	33	0.00	30
V_{anx}	-0.08	16	-0.03	18	-0.02	9	0.01	26
V_{aer}	0.19	8	-0.30	4	-0.04	8	0.21	4
K_{Iaanx}	0.12	13	-0.04	17	0.00	27	0.01	22
K_{Iamax}	0.35	3	-0.41	2	0.01	19	0.67	1
S_{Osat}	0.14	11	-0.16	9	0.00	23	0.00	32
Q_r	0.06	18	-0.06	14	-0.01	15	0.04	14
Q_{intr}	0.05	22	0.03	21	0.00	32	0.02	19

The detailed interpretation of the sensitivity analysis results leads to following conclusions:

- Effluent nitrate: by far the most important source of uncertainty determining the variance in the effluent nitrate are the influent fractions, especially the non-biodegradable and biodegradable fractions.
- Sludge production: Firstly, only 4 parameters had an SRC higher than 0.1: $\{X_{2TSS}, f_{XI}, Y_H, f_P\}$. This means that varying ash content and influent insoluble solids (the X_{2TSS} and f_{XI}) result in variations in the sludge production and hence the SRT in the system, which is known from process engineering knowledge and confirmed hereby by formal statistical analysis. Next the degree of linearization (R2) is ca 1.00 meaning that the sludge production can actually be predicted by a linear model in the plant. Therefore the system of coupled ordinary differential equations can be replaced by linear algebraic equations which significantly reduces computational effort.
- Effluent ammonium: The ash content of the influent wastewater and the solids in the tank (X_{2TSS}) along with the influent inert particulate fraction (f_{XI}) were found the most influential on the effluent ammonium concentration. This can be explained by the effect of these two parameters on the system SRT (sludge production, see above), hence a decrease in the system SRT will cause a decrease in the amount of nitrifying organisms, which consequently leads to higher effluent ammonium concentration. These results are expected as the BSM1 plant is designed to be limited by its nitrification capacity.
- Aeration energy demand: The following parameters were found to be significant: $\{K_{1a_{max}}, V_{aer}, f_{XI}, Y_H, X_{2TSS}, i_{XB}, f_{SS}, n_{hyd}, f_P, f_{XBH}, K_{OH}, b_H\}$. This shows that aeration energy demand is directly associated to the sludge production and nitrification, i.e. less aeration with more sludge production (less COD degradation) and more aeration with lower ammonium in effluent. Also the aeration system parameters of the plant (e.g maximum mass transfer coefficient) are found to be important.

In summary, sensitivity analysis based on variance decomposition (such as SRC) offers new ways of extracting information that can help design engineers deal with uncertainties in engineering projects. For example, the sensitivity analysis results explained – in accordance with process engineering knowledge – the major contributing parameters to the uncertainty in plant performance. This information complements the uncertainty analysis of a modelling study and provides the process engineer with the critical information needed to devise ways to reduce the uncertainty to acceptable levels. Second, the methods are well established, while performing this analysis may be computationally costly but in light of fast developments in IT should become trivial.

Case study 2: Application of sensitivity analysis to fine-tuning of the fuzzy-controller

The Morris method was applied to a different number of elementary effects, r , until the sensitivity of parameters remained more or less stable. As a result, $r=60$ was selected as the optimal number of repetitions for this case study. The overall model evaluation costs were therefore 1080 simulations ($=r*(k+1)$, $k=17$). These results are in contrast with previous applications of the Morris method since most of these studies used a low repetition number, e.g. $r=(10\sim20)$ (Campolongo et al, 2007). As these results indicate, r has a significant effect on the identified parameter sensitivity, particularly for a low value of r , (lower than $r=30$, in this case study). This fact implies the necessity of finding out the optimal repetition number for SEE_{jk} calculations (r). A non-optimal selection of r would lead to Type II error, failing in the identification of a parameter of considerable influence in the model and Type I Error, as well, considering a factor as significant when it is not. For instance, in this case study, for a sample size of $r=10$ the parameter RT (response time) was characterised by a low mean and low standard deviation. In contrast, the results for the optimal sample size showed that this

parameter presents a considerable effect in the output variables as was expected from practical experience.

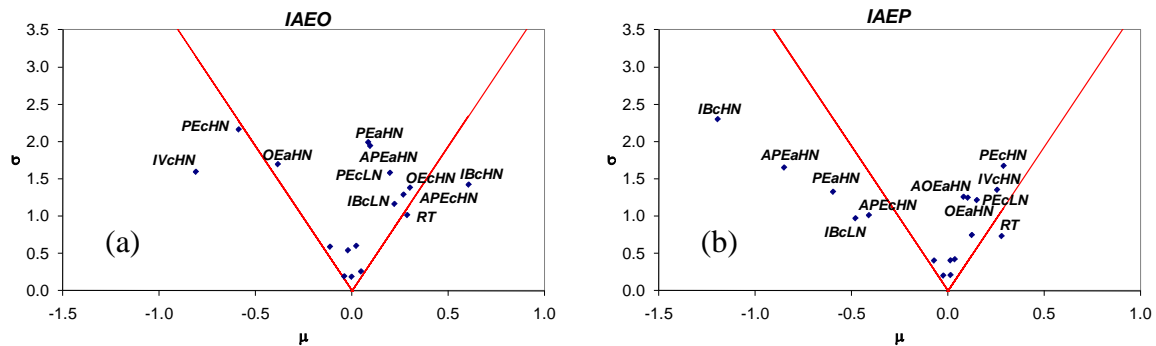


Figure 2. μ versus σ , for $r_{\text{opt}} = 60$. Lines correspond to $\mu_i = \pm 2\text{SEM}_i$. (a) *IAEO* output variables; (b) *IAEP* output variable

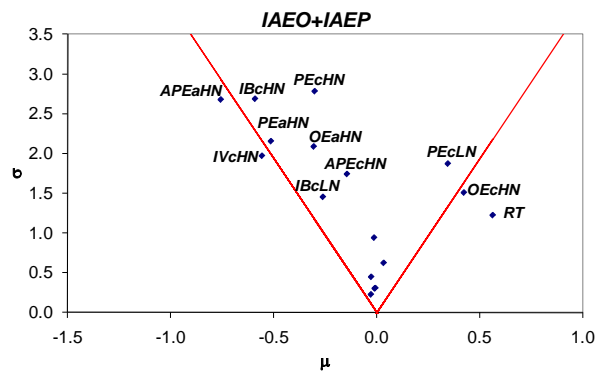


Figure 3. μ versus σ , for $r_{\text{opt}} = 60$ for the weighted contribution of *IAEO* and *IAEP*

Compared to the results obtained in previous work (Ruano et al., 2009), in which local sensitivity analysis was used to find significant parameters, the following could be said: (i) significant parameters identified in the local sensitivity analysis agreed mostly with those identified by the method of Morris, e.g. OECHN and RT parameters, (ii) only one parameter identified as influential in the local sensitivity analysis is found to be non-influential according to the Morris screening study (*AOEaHN*, i.e. High Negative amplitude of the accumulated oxygen error). Hence these results demonstrate that global methods in particular Morris Screening are more resilient to type II error, i.e. identifying non-influential parameters as influential. Hence it is recommended for use in identifiability problems.

However one caveat has to be mentioned when using Morris screening method, which has to do with the selection of a proper repetition number of EE_i calculations (r_{opt}). Probably, a high value of the parameter r will be needed when either a highly nonlinear model is used, or a large input uncertainty is defined. Working with a non proper sample size (r) could lead to Type I and Type II error. It thus comes with a slightly higher computational cost, which is increasingly feasible to do. We recommend Morris screening as an efficient and promising method for sensitivity analysis in the wastewater modelling community for applications ranging from model calibration to controller fine-tuning applications.

Concluding remarks

This paper presented two applications of global sensitivity analysis dealing with two case studies: plant design versus plant operation (fine-tuning of controllers in particular). The results from each application showed that variance based decomposition methods are well established albeit with a manageable computational cost. The results supplemented with process engineering knowledge provide valuable insights into the engineering problems at hand thereby help engineers in doing their day-to-day works such as checking the robustness of plant design or helping to fine-tune a controller applied to a plant.

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